

QUANTUM ENTANGLEMENT AND APPROXIMATION BY POSITIVE MATRICES

XIAOFEN HUANG AND NAIHUA JING*

ABSTRACT. We give an exact solution to the nonlinear optimization problem of approximating a Hermitian matrix by positive semi-definite matrices. Our algorithm was then used to judge whether a quantum state is entangled or not. We show that the exact approximation of a density matrices by tensor product of positive semi-definite operators is determined by the additivity property of the density matrix.

1. INTRODUCTION

Quantum entanglement is one of the most interesting features in quantum computation [20, 23] as it is vital for quantum dense coding, quantum error-correcting codes, teleportation and also responsible for fast quantum algorithms. Much efforts have been made to find criteria for quantum separability: the Bell inequalities [3], PPT (positive partial transposition) [23], reduction criterion [5, 12], majorization criterion [22], entanglement witnesses [16, 26, 19], realignment [24, 6] and generalized realignment methods [1]. Nevertheless the problem is still not fully solved except for lower rank cases [16, 2, 7].

In [8] we proposed a new method to judge if a density matrix is separable. We first decompose the density matrix as a tensor product of hermitian matrices, and then we reduce the separability problem to that of finding when the hermitian matrix becomes positive semi-definite. The strategy was to solve the separability by two steps: first one finds a tensor decomposition of the density matrix by hermitian matrices, and then one approximates the hermitian matrices by positive semi-definite matrices if possible. Although it was proved that a density matrix is separable if and only if the separability indicator is non-negative, it is highly nontrivial to actually compute this indicator. In this sense the method is also similar to many of its predecessors.

In the current paper we approach the question from a new angle by giving an algorithm to compute the closest positive semi-definite matrix to any given hermitian matrix. It is noted that this optimization is not a linear problem so the usual QR decomposition in [15] does not work. By general theory of convex sets the existence of the minimum is guaranteed but it is

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*Corresponding author.

nontrivial to find the exact solution due to the nonlinearity. In this paper we first solve this optimization problem exactly using matrix theory. This paves the way for us to attack the main problem of separability by directly looking for an optimal approximation to a sum of matrices by positive semi-definite matrices.

It turns out that the exact solution in the most important case can be solved by Lie theoretic techniques. First we show that a Hermitian matrix with two commuting summands can be approximated term by term. Next we prove that if the summands of a Hermitian matrix can be simultaneously made to upper triangular matrices, then the exact approximation by positive semi-definite matrix can be done term by term. Our method provides a direct way to approximate the hermitian matrix by positive semi-definite matrices and thus the separability problem can be solved theoretically in this sense.

It is interesting to note that similar (but stronger constrained) matrix approximation also appears in finance, image processing, data mining, and other areas such as resource allocation and industrial process monitoring [25, 28, 4]. Most methods used in these problems are numerical algorithms that only give an approximation to the solution. In some sense our results also provide the first exact and analytical method in this direction, and we also hope that conversely some of the numerical algorithms may be useful in quantum entanglements.

2. APPROXIMATION BY POSITIVE DEFINITE MATRICES

Let A be an $n \times n$ Hermitian matrix, and let Q be a unitary matrix such that $A = QDQ^\dagger$, where $D = \text{diag}(\alpha_1, \dots, \alpha_n)$ and \dagger is conjugation and transposition. The signature (p, q) of A (cf. [18]) is defined by $p + q = \text{rank}(A)$. We can permute the columns of the matrix Q so that the eigenvalues of A are arranged in the following order:

$$\alpha_1 \geq \dots \geq \alpha_p > 0 > \alpha_{p+1} \geq \dots \geq \alpha_{p+q}, \alpha_{p+q+1} = \dots = \alpha_n = 0.$$

We further define

$$(1) \quad A = A_+ - A_-,$$

where $A_\pm = QD_\pm Q^\dagger$, and

$$\begin{aligned} D_+ &= \text{diag}(\alpha_1, \dots, \alpha_p, 0, \dots, 0) \\ D_- &= \text{diag}(0, \dots, 0, -\alpha_{p+1}, \dots, -\alpha_{p+q}, 0, \dots, 0) \end{aligned}$$

formed by positive (negative) eigenvalues respectively. We remark that our definition of the positive and negative semi-definite parts of A is independent from our choice of Q . In general, if A is diagonalized by a unitary matrix Q as follows:

$$A = QDQ^\dagger = Q\text{diag}(\alpha_1, \dots, \alpha_n)Q^\dagger,$$

then we have

$$A_{\pm} = Q \text{diag}(\alpha_1^{\pm}, \dots, \alpha_n^{\pm}) Q^{\dagger}, \quad \alpha_i^{\pm} = \frac{|\alpha_i| \pm \alpha_i}{2}.$$

It is clear that A is positive semi-definite if and only if all eigenvalues of A are non-negative. Therefore both A_{\pm} are positive semi-definite matrices. It is easy to see that the decomposition (1) of A into a difference of positive semi-definite matrices is unique up to positive definite matrices, i.e., if $A = A'_+ - A'_-$, where A'_{\pm} are positive semi-definite, then $A_{\pm} = A'_{\pm} + P$ with a positive semi-definite matrix P .

If A and B are commuting positive semi-definite matrices, so is their product. If they are not commutative, then AB is in general not a positive semi-definite matrix, as AB may not even be hermitian.

Lemma 2.1. *Let A and B be positive semi-definite Hermitian matrices, then the eigenvalues of AB are all non-negative.*

Proof. If A is invertible, and let λ be an eigenvalue of AB , then for some vector $x \neq 0$,

$$ABx = \lambda x.$$

Hence $Bx = \lambda A^{-1}x$. Note that both A^{-1} and B are positive, so

$$x^{\dagger} Bx = \lambda x^{\dagger} A^{-1}x > 0,$$

Subsequently $\lambda > 0$. In general, if A is singular, then for any $\epsilon > 0$ the matrix $A + \epsilon I$ is positive definite. Therefore any eigenvalue $\lambda = \lambda(\epsilon)$ of $(A + \epsilon I)B$ is positive. Letting $\epsilon \rightarrow 0$, we see that $\lim_{\epsilon \rightarrow 0} \lambda \geq 0$, i.e. any eigenvalue of AB is non-negative. \square

For any matrix A , the Frobenius norm is defined to be $\|A\|_F = (\text{tr}(AA^{\dagger}))^{1/2}$, which is also equal to the sum of squares of singular values of A .

Theorem 2.2. *Let A be an $n \times n$ hermitian matrix, then for any positive semi-definite matrix B we have*

$$(2) \quad \|A - B\|_F \geq \|A_{-}\|_F$$

with equality when $B = A_{+}$. i.e. the closest positive semi-definite matrix to A is given by A_{+} .

Proof. Omitting the subscript in the Frobenius norm, we have for any positive semi-definite matrix B

$$\begin{aligned} \|A - B\|^2 &= \text{tr}(A - B)^2 = \text{tr}(A^2) - 2\text{tr}(AB) + \text{tr}(B^2) \\ &= \text{tr}(A^2) + 2\text{tr}(A_{-}B) + \text{tr}(B^2) - 2\text{tr}(A_{+}B) \\ &= \text{tr}(A^2) + 2\text{tr}(A_{-}B) + \text{tr}(B - A_{+})^2 - \text{tr}(A_{+}^2) \end{aligned}$$

by using $\text{tr}(AB) = \text{tr}(BA)$ and completing square. Since B and A_{\pm} are positive semi-definite, then $\text{tr}(A_{-}B) \geq 0$ for any B by Lemma 2.1. Therefore,

it follows that for any positive semi-definite matrix B

$$\begin{aligned}\|A - B\|^2 &\geq \text{tr}(A^2) + \text{tr}(B - A_+)^2 - \text{tr}(A_+^2) \\ &= \|A\|^2 - \|A_+\|^2 + \|B - A_+\|^2 \\ &\geq \|A\|^2 - \|A_+\|^2\end{aligned}$$

where the equality is obtained when $B = A_+$. \square

We remark that similar (Toeplitz and/or correlation matrix) approximation with stronger constraints has been studied in finance and image processing [25, 28]. Our result is more general and stronger in the sense that we do not require that the matrix to be either Toeplitz or correlation matrix (real positive definite with unit diagonal). Furthermore our result is analytical and exact, as no numerical approximation is needed for the solution.

Corollary 2.3. *Let A and B be any two Hermitian matrices, then for any positive semi-definite matrix C of the same size as $A \otimes B$, we have*

$$\|A \otimes B - C\|_F \geq \|(A \otimes B)_-\|_F = \|A_+ \otimes B_- + A_- \otimes B_+\|_F.$$

The equality holds when $C = (A \otimes B)_+ = A_+ \otimes B_+ + A_- \otimes B_-$.

Proof. It is enough to show that $(A \otimes B)_\pm = \sum_\epsilon A_\epsilon \otimes B_{\pm\epsilon}$, where $\epsilon = +, -$. Suppose A and B are diagonalized by Q_1 and Q_2 respectively:

$$\begin{aligned}A &= Q_1 D_1 Q_1^\dagger = Q_1 \text{diag}(\alpha_1, \dots, \alpha_m) Q_1^\dagger, \\ B &= Q_2 D_2 Q_2^\dagger = Q_2 \text{diag}(\beta_1, \dots, \beta_n) Q_2^\dagger\end{aligned}$$

then we have

$$A \otimes B = (Q_1 \otimes Q_2)(D_1 \otimes D_2)(Q_1 \otimes Q_2)^\dagger$$

As the eigenvalues σ of $A \otimes B$ are $\lambda_i \beta_j$, thus

$$\begin{aligned}\sigma_{ij}^+ &= \alpha_i^+ \beta_j^+ + \alpha_i^- \beta_j^-, \\ \sigma_{ij}^- &= \alpha_i^+ \beta_j^- + \alpha_i^- \beta_j^+, \\ \sigma_{ij}^0 &= \alpha_i^0 \beta_j + \alpha_i \beta_j^0.\end{aligned}$$

Since the zero eigenvalues do not contribute to the decomposition, we have that $(A \otimes B)_+ = A_+ \otimes B_+ + A_- \otimes B_-$, and $(A \otimes B)_- = A_+ \otimes B_- + A_- \otimes B_+$. \square

3. SUMS OF MATRICES AND ESTIMATES

It appears that the decomposition of the Hermitian matrix A into a sum of two Hermitian matrices B, C has a close relationship to our problem. This problem has a much longer history in mathematics.

Horn [11] defines the following concept for the Hermitian matrices. Let A and B be two $n \times n$ matrices with eigenvalues α_i and β_i . For any subset I we denote $|I| = \sum_{i \in I} i$. The set T_r^n of triples (I, J, K) of subsets of $\{1, \dots, n\}$ of the same cardinality r is defined by first setting

$$U_r^n = \{(I, J, K) \mid |I| + |J| = |K| + r(r+1)/2\},$$

then define $T_1^n = U_1^n$ and in general

$$T_r^n = \{(I, J, K) \in U_r^n \mid \text{for all } p < r \text{ and all } (F, G, H) \in U_p^n \\ \sum_{f \in F} i_f + \sum_{g \in G} j_g \leq \sum_{h \in H} k_h + p(p+1)/2\},$$

The following characterization of eigenvalues α, β, γ of $C = A + B$ is proved in [9].

Theorem 3.1. (Horn's conjecture) *A triple (α, β, γ) occurs as eigenvalues of A, B, C such that $C = A + B$ if and only if $|\alpha| + |\beta| = |\gamma|$ and inequalities*

$$\sum_{k \in K} \gamma_k \leq \sum_{i \in I} \alpha_i + \sum_{j \in J} \beta_j$$

hold for all triple (I, J, K) in T_r^n for all $r < n$.

The special case of $r = 1$ is Weyl's inequality:

$$\gamma_{i+j-1} \leq \alpha_i + \beta_j$$

Since $|\gamma| = |\alpha| + |\beta|$, we also have

$$\sum_{k \in K^c} \gamma_k \geq \sum_{i \in I^c} \alpha_i + \sum_{j \in J^c} \beta_j$$

A practical bound is the following:

$$\max_{i+j=n+k} \alpha_i + \beta_j \leq \gamma_k \leq \min_{i+j=k+1} \alpha_i + \beta_j$$

Apply these results to our situation, we then get the following:

Theorem 3.2. *Let A be a density matrix over the Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. Suppose $A = \sum_i B_i \otimes C_i$, then we have*

$$\|A - A_+\|_F \leq \sum_i \|B_i - (B_i)_+\| \cdot \|C_i - (C_i)_+\|$$

4. LIE ALGEBRAS AND APPROXIMATION OF SUMMATIONS

As the Hermitian decomposition of the density matrix A is a summation, one hopes to check its separability by demonstrating that each summand can be expressed by tensor products of positive semi-definite matrices.

The main problem is to estimate the error given by term by term approximation. Suppose that A and B are two Hermitian matrices we would like to estimate the norm $\|A + B - A_+ - B_+\|$.

Lemma 4.1. *Let A and B are two commuting Hermitian matrices, then*

$$(A + B)_+ \leq A_+ + B_+ \\ (A + B)_- \leq A_- + B_-$$

Proof. Since A and B are commuting, they can be diagonalized simultaneously by a unitary matrix Q . In other words we have

$$\begin{aligned} A &= QD_AQ^\dagger = A_+ - A_- = Q(D_A)_+Q^\dagger - Q(D_A)_-Q^\dagger \\ B &= QD_BQ^\dagger = B_+ - B_- = Q(D_B)_+Q^\dagger - Q(D_B)_-Q^\dagger \end{aligned}$$

thus,

$$\begin{aligned} A + B &= Q(D_A + D_B)Q^\dagger \\ &= Q((D_A)_+ + (D_B)_+)Q^\dagger - Q((D_A)_- + (D_B)_-)Q^\dagger, \end{aligned}$$

which implies that $(A + B)_+ = A_+ + B_+$ and $(A + B)_- = A_- + B_-$. \square

Theorem 4.2. *Let A_i (resp. B_i) be set of commuting positive semi-definite Hermitian matrices of the same size, then for any positive definite matrix C of the same size as $A_i \otimes B_i$ we have*

$$\left\| \sum_i A_i \otimes B_i - C \right\|_F \geq \left\| \sum_i \{(A_i)_+ \otimes (B_i)_- + (A_i)_- \otimes (B_i)_+\} \right\|_F,$$

where the equality holds when

$$C = \sum_i (A_i \otimes B_i)_+ = \sum_i \{(A_i)_+ \otimes (B_i)_+ + (A_i)_- \otimes (B_i)_-\}.$$

We remark that the condition that A and B are commuting with each other is also necessary for the equality in the theorem to hold. The following result is quoted from standard books on Lie algebras [10].

Proposition 4.3. *(Lie's theorem) Let L be any solvable subalgebra of the general linear Lie algebra, then the matrices of L relative to a suitable basis of V are upper triangular. Furthermore, one can adjust the basis to be orthonormal.*

We remark that the last statement is due to the fact that the transition matrix in Gram-Schmidt process is upper triangular. Now we suppose that there exists a unitary matrix Q such that both A and B are upper-triangularized as follows:

$$A = Q\Lambda_1Q^\dagger, B = Q\Lambda_2Q^\dagger,$$

where Λ_i are upper-triangular. If A and B are hermitian, then $\Lambda_i^\dagger = \Lambda_i$, which forces Λ_i to be diagonal. Then A and B are actually commuting with each other, subsequently $(A + B)_\pm = A_\pm + B_\pm$. So in this context the additivity seems to be not too far away from commutativity.

Theorem 4.2 gives the closest approximation to a two-partite density operator by the tensor operator of non-negative operators, however one has to fit the approximation under the constraint of unit trace. We hope that further studies can answer this question.

5. CONCLUSION

Matrix approximation is an old problem in mathematics with applications in physics, finance, and computer sciences. In this paper we have completely solved the optimization problem to approximate any Hermitian matrix by positive semi-definite matrices. The solution is shown to be given by the spectral decomposition of the concerned matrix. We apply this result to density matrices and obtain useful approximation by tensor product of density matrices using Lie theoretic techniques. Our results also open possible deep connection among quantum entanglement, data mining and signal procession.

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SCHOOL OF MATHEMATICS AND STATISTICS, HAINAN NORMAL UNIVERSITY, HAIKOU,
HAINAN 571158, CHINA

E-mail address: `huangxf1206@gmail.com`

SCHOOL OF SCIENCES, SOUTH CHINA UNIVERSITY OF TECHNOLOGY, GUANGZHOU
510640, CHINA AND DEPARTMENT OF MATHEMATICS, NORTH CAROLINA STATE UNI-
VERSITY, RALEIGH, NC 27695, USA

E-mail address: `jing@math.ncsu.edu`